A Mechanism of Spin-Triplet Superconductivity in Hubbard Model on Triangular Lattice: Application to UNi_2Al_3

Yunori NISIKAWA* and Kosaku YAMADA

Department of Physics, Kyoto University, Kyoto 606-8502

We discuss the possibility of spin-triplet superconductivity in a two-dimensional Hubbard model on a triangular lattice within the third-order perturbation theory. When we vary the symmetry in the dispersion of the bare energy band from D_2 to D_6, spin-singlet superconductivity in the D_2-symmetric system is suppressed and we obtain spin-triplet superconductivity in near the D_6-symmetric system. In this case, it is found that the vertex terms, which are not included in the interaction mediated by the spin fluctuation, are essential for realizing the spin-triplet pairing. We point out the possibility that obtained results correspond to the difference between the superconductivity of UNi_2Al_3 and that of UPd_2Al_3.

KEYWORDS: spin-triplet superconductivity, two-dimensional Hubbard model on triangular lattice, third-order perturbation theory, vertex correction, UNi_2Al_3, UPd_2Al_3

Heavy-fermion superconductors have attracted much interest since spin-triplet superconductivity has been reported in these compounds. Respective isostructual hexagonal $PrNi_2Al_3$-type heavy-fermion compounds, UPd_2Al_3 and UNi_2Al_3, were found to be superconductors with $T_c \simeq 2$ and 1K, respectively. Their superconducting states coexist with antiferromagnetic long-range orders with $T_N = 14.3$ and 4.5K, respectively. The properties of magnetism and superconductivity are different in each compound. UPd_2Al_3 orders in an antiferromagnetic long-range structure with a commensurate wave vector $\mathbf{k} = (0, 0, 0.5)$ and has a large ordered magnetic moment $\mu = 0.85\mu_B$ on uranium atoms. UNi_2Al_3 orders in a spin-density wave (SDW) with an incommensurate wave vector $\mathbf{k} = (H \pm 0.61, 0, 0.5)$ and has a tiny magnetic moment of $0.2\mu_B$ whose magnitude is modulated within the basal plane. Regarding the superconducting properties, various experiments suggest that UPd_2Al_3 is a spin-singlet d-wave superconductor with a line-node gap. On the other hand, spin-triplet superconductivity in UNi_2Al_3 has been revealed by the NMR measurement recently.[1] We have proposed a theory of the superconductivity in UPd_2Al_3.[2] Therefore, we have to explain the mechanism of the spin-triplet superconductivity in UNi_2Al_3 and the difference between the superconducting state of UNi_2Al_3 and that of UPd_2Al_3 from the same viewpoint as that of our previous work, although the detailed electronic structure of UNi_2Al_3 has not been investigated yet. Motivated by the point mentioned above, we discuss the possibility of spin-triplet superconductivity in a two-dimensional Hubbard model on a triangular lattice, as a first step. In the case of spin-

*E-mail address:nisikawa@scphys.kyoto-u.ac.jp

triplet superconductor Sr_2RuO_4, Nomura and Yamada have recognized that the momentum and frequency dependence of the effective interaction between electrons, which is not included in the interaction mediated by the spin fluctuation, is essential for realizing the spin-triplet pairing and they have explained the superconducting mechanism within the third-order perturbation theory (TOPT).[3] The perturbation approach is sensitive to the dispersion of the bare energy band, by its nature. It implies that the lattice structures and the band filling play essential roles in the calculation of superconducting transition temperature T_c. Therefore, it is important to evaluate superconducting transition temperature T_c on the basis of the detailed electronic structure in each system. In this paper, we also calculate T_c of spin-triplet superconductivity in a two-dimensional Hubbard model on a triangular lattice within the TOPT. In a similar model, Kuroki and Arita have proposed that spin-fluctuation-mediated spin-triplet superconductivity can be realized in their model with disconnected Fermi surfaces, by using fluctuation-exchange approximation (FLEX).[4] However, as mentioned later, our proposed mechanism of spin-triplet superconductivity is completely different from their proposed mechanism.

We start from the quasi-particle state according to the discussion of our previous work.[5] We write the model Hamiltonian as follows:

$$H = H_0 + H_1, \tag{1}$$

$$H_0 = \sum_{\mathbf{k},\sigma} (\epsilon(\mathbf{k}) - \mu)\, a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}, \tag{2}$$

$$H_1 = \frac{U}{2N} \sum_{\sigma\neq\sigma'} \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4} a^\dagger_{\mathbf{k}_1\sigma} a^\dagger_{\mathbf{k}_2\sigma'} a_{\mathbf{k}_3\sigma'} a_{\mathbf{k}_4\sigma}, \tag{3}$$

where $a^\dagger_{\mathbf{k}\sigma}(a_{\mathbf{k}\sigma})$ is the creation(annihilation) operator for the electron with momentum $\mathbf{k}$ and spin index σ; $\epsilon(\mathbf{k})$ and μ are the dispersion of the bare energy band on a two-dimensional triangular lattice and the chemical potential, respectively. The sum over $\mathbf{k}$ indicates taking summation over a primitive cell of the inverse lattice. In the above equations, we have rescaled the length, energy, temperature and time by $a, t, \frac{t}{k_B}, \frac{\hbar}{t}$. (where a, t, k_B and $\hbar$ are the lattice constant, the nearest neighbor hopping integrals, Boltzmann constant and Planck constant divided by 2π, respectively)

We calculate T_c by solving Éliashberg's equation (Fig. 1). In the equation, the normal self-energy and the effective interaction are obtained within the third-order perturbation with respect to U(Fig. 2). The diagrams enclosed by a dashed line in Fig. 2(b) are the vertex correction terms which are not direct contributions from spin fluctuations. The other diagrams are included in RPA. We call the latter 'RPA-like diagrams' in this paper. In Fig. 2(b), we omit writing the diagrams given by turning the vertex correction terms in Fig. 2(b) upside down.

Our model parameters are the dispersion $\epsilon(\mathbf{k})$ of the bare energy band on a two-

dimensional triangular lattice, the electron number n per one spin site and the Coulomb repulsion U. Regarding the dispersion of the bare energy band, we consider the following dispersions of the bare energy band.

At first, we consider the following:

$$\epsilon_{\mathrm{D}_2}(\mathbf{k}, t_{\mathrm{m}}) = -4\cos(\frac{\sqrt{3}}{2}k_x)\cos(\frac{1}{2}k_y) - 2t_{\mathrm{m}}\cos(k_y); t_{\mathrm{m}} \neq t(=1). \tag{4}$$

$\epsilon_{\mathrm{D}_2}(\mathbf{k}, t_{\mathrm{m}})$ exhibits only the D_2-symmetry because of $t_{\mathrm{m}} \neq 1$ (Fig. 3(a)). In the case of spin-singlet superconductor UPd_2Al_3, we adopted the above dispersion of the bare energy band in the previous work.[2] In the previous work, we have considered only the nearest neighbor hopping integrals and we have assumed that the value of hopping integral t_{m} along the magnetic moment is different from the value of other hopping integrals t, because the superconductivity of UPd_2Al_3 is realized in the antiferromagnetic state. Thus we have included the effect of the antiferromagnetic order in the difference between t_{m} and t. We have also determined the values so as to reproduce the considered Fermi sheet which is obtained by the band calculation and is not of D_6-symmetry, reflecting the antiferromagnetic structure. We have concluded that the main origin of the superconductivity is the momentum dependence of the spin fluctuations which stems from the shape of our considered Fermi sheet which undergoes symmetry breakdown($\mathrm{D}_6 \rightarrow \mathrm{D}_2$-symmetry) due to the antiferromagnetic order and then possesses nesting properties. In the present paper, we investigate how superconducting states change when we vary t_{m}(symmetry in the system) from $t_{\mathrm{m}} \neq 1(\mathrm{D}_2)$ to $t_{\mathrm{m}} = 1(\mathrm{D}_6)$. We also investigate the possibility of spin-triplet superconductivity near the previous model of UPd_2Al_3. Then we discuss a possible model of UNi_2Al_3, although the detailed electronic structure of UNi_2Al_3 has not been investigated yet.

Next we consider D_6-symmetric dispersions of the bare energy band (*i.e*, dispersions of the bare energy band without anisotropic nature in the hopping integrals). In this paper, we consider the nearest neighbor hopping model. We also consider the following dispersion of the bare energy band:

$$\epsilon_{\mathrm{D}_6}(\mathbf{k}) = \epsilon_{\mathrm{D}_2}(\mathbf{k}, 1). \tag{5}$$

To satisfy Luttinger's theorem, that is, the conservation law of particle number, we adjust the chemical potential μ by using the secant method. To solve Éliahberg's equation by using the power method algorithm, we have to calculate the summation over the momentum and the frequency space. Since all summations are in the convolution forms, we can carry them out by using the algorithm of the fast Fourier transformation. For the frequency, irrespective of the temperature, we have 1024 Matsubara frequencies. Therefore, we calculate throughout in the temperature region $T \geq T_{\mathrm{lim}}$, where T_{lim} is the lower limit temperature for reliable numerical calculation, which is estimated to be about $3.0 \times 10^{-3} (> \Delta\epsilon/(2\pi \times 1024) \simeq 1.4 \times 10^{-3})$, where $\Delta\epsilon$ is the bandwidth; we divide a primitive cell into 128×128 meshes.

Table I. Irreducible representations of D_2

Irreducible representation	Parity	Basis functions (maximum wavelength in **k**-space)
A	even	1
B_1	even	$c_1^{(1)} - c_2^{(1)}$
B_2	odd	$s_1^{(1)} + s_2^{(1)}, s_3^{(1)}$
B_3	odd	$s_1^{(1)} - s_2^{(1)}$

To investigate how superconducting states change when we vary $t_{\rm m}$ (symmetry in the system) from $t_{\rm m} \neq 1(D_2)$ to $t_{\rm m} = 1(D_6)$, we calculate the eigenvalues of Éliahberg's equation for various $t_{\rm m}(0.75 \sim 0.99)$ and n, starting from the model parameters of our previous work ($\epsilon_{D_2}(\mathbf{k}, t_{\rm m}), t_{\rm m} = 0.75, n = 0.572$). In this calculation, we select the Coulomb repulsion $U = 7.5$. In the case of the D_2-symmetric system, we can classify the eigenvalues of Éliahberg's equation according to the irreducible representations of D_2. D_2 has four irreducible representations (see Table I).

The short notations $s_j^{(i)}$ and $c_j^{(i)}$ in Tables I and II mean that $s_j^{(i)} \equiv \sin(\mathbf{R}_j^{(i)} \cdot \mathbf{k})$ and $c_j^{(i)} \equiv \cos(\mathbf{R}_j^{(i)} \cdot \mathbf{k})$, where $\mathbf{R}_j^{(i)}$ is defined in Fig. 3(b).

The eigenvalues which belong to A or B_1 correspond to spin-singlet states. The eigenvalues which belong to B_2 or B_3 correspond to spin-triplet states. Based on the values of our parameters, in the case of spin-singlet states, the maximum eigenvalue belongs to B_1 and in the case of spin-triplet states, the maximum eigenvalue belongs to B_2.

The results are shown in Fig. 4. From this figure, the following facts are evident.

In the case of $n = 0.572$ and $t_{\rm m} = 0.75$, the spin-singlet state is most stable. We have pointed out that this spin-singlet state corresponds to that of UPd_2Al_3 in our previous work. When we vary $t_{\rm m}$ (symmetry in the system) from $t_{\rm m} = 0.75(D_2)$ to $t_{\rm m} = 1(D_6)$, at the same time, the anisotropic nature in spin fluctuation is suppressed. In this case, the spin-singlet state is suppressed because the main origin of the d-wave superconductivity is the momentum and frequency dependence of spin fluctuations as we have pointed out in our previous work, and we can see that spin-triplet states have the tendency to emerge.

Next, we consider D_6-symmetric dispersions $\epsilon_{D_6}(\mathbf{k})$ of the bare energy band and calculate $T_{\rm c}$ for some model parameters U and n. In the case of the D_6-symmetric system, we can classify the eigenvalues of Éliahberg's equation according to the irreducible representations of D_6. D_6 has six irreducible representations (see Table II).

The eigenvalues which belong to A_1, A_2 or E_2 correspond to spin-singlet states. The eigenvalues which belong to B_1, B_2 or E_1 correspond to spin-triplet states. Based on the values of our parameters, the maximum eigenvalue belongs to E_1 which corresponds to a spin-triplet state.

Table II. Irreducible representations of D_6

Irreducible representation	Parity	Basis functions (maximum wavelength in **k**-space)
A_1	even	1
A_2	even	$c_1^{(4)} - c_2^{(4)} + c_3^{(4)} - c_4^{(4)} + c_5^{(4)} - c_6^{(4)}$
E_2	even	$\{c_1^{(1)} - c_2^{(1)}, c_1^{(1)} + c_2^{(1)} - 2c_3^{(1)}\}$
B_1	odd	$s_1^{(1)} + s_2^{(1)} + s_3^{(1)}$
B_2	odd	$s_1^{(2)} + s_2^{(2)} + s_3^{(2)}$
E_1	odd	$\{s_1^{(1)} - s_2^{(1)}, s_1^{(1)} + s_2^{(1)} - 2s_3^{(1)}\}$

The dependences of T_c on U and n are shown Fig. **??**. On the basis of these results, we can point out the following findings. For large U, high T_c values are obtained for all parameters.

When we increase the electron density n for the fixed valued Coulomb repulsion U and the Fermi level becomes close to the van Hove singularity (whose results are not presented in this paper), then high T_c values are obtained.

To examine how the vertex corrections influence T_c, we also tried to calculate T_c by including only the RPA-like diagrams but we could not find any finite value of T_c within the precision of our numerical calculations. Therefore, we can calculate only the eigenvalue by including only the RPA-like diagrams at T_c obtained by using the TOPT.

From these results, it is found that the vertex terms, which are not included in the interaction mediated by the spin fluctuation, are essential for realizing the spin-triplet pairing.

In this paper, we have discussed the possibility of spin-triplet superconductivity in a two-dimensional Hubbard model on a triangular lattice within the TOPT and we have obtained spin-triplet superconducting states in near a D_6-symmetric system. In this case, the vertex correction terms play an essential role in obtaining the spin-triplet superconducting states. This is the same result that Nomura and Yamada have obtained in the investigation of the mechanism of spin-triplet superconductor Sr_2RuO_4 within the TOPT, as we have mentioned above. Jujo *et al.* have investigated the mechanism of the spin-singlet superconductivities in organic superconductors κ-type (BEDT-TTF)$_2$X within the TOPT and FLEX.[6] They have compared the results between the TOPT and FLEX, and have pointed out that the vertex correction terms (which are also not included in the FLEX) have a crucial effect on the calculation of T_c for strongly frustrated systems. Therefore, our presented results are consistent with the above two results. Recently, Nisikawa *et al.* have discussed the spin-singlet superconductivity in $CeIr_xCo_{1-x}In_5$ within the TOPT and have pointed out that the vertex correction terms are important to explain the x-dependence of T_c.[5] The findings described above suggest that the calculations of T_c, which include only the spin fluctuation terms, are questionable and should be carefully performed with vertex corrections.

UNi_2Al_3 and UPd_2Al_3 undergo superconducting transition below the Néel temperature. Therefore, the symmetry in the itinerant electron system under the antiferromagnetic structure is one of the important matters to consider in investigating the mechanism of superconductivity. In the case of UPd_2Al_3, the symmetry in the itinerant electron system is not of hexagonal symmetry, reflecting the effect of the antiferromagnetic structure with a large ordered magnetic moment $\mu = 0.85\mu_B$ on uranium atoms, and we have treated this by considering the anisotropic hopping integral $t_m \neq 1$. In this context, the symmetry in the itinerant electron system of UNi_2Al_3 may be more isotropic than the symmetry in that of UPd_2Al_3 because of a reflecting incommensurate SDW order with a tiny moment of $0.2\mu_B$, although the detailed electronic structure of UNi_2Al_3 has not been investigated yet. Therefore, we assume that $t_m \simeq 1$ in the case of UNi_2Al_3. Based on the hypothesis mentioned above, our results seem to explain not only the mechanism of spin-triplet superconductivity in UNi_2Al_3 but also the difference between the superconductivity of UNi_2Al_3 and that of UPd_2Al_3 because the spin-singlet superconductivity in the D_2-symmetric system($t_m \neq 1$) is suppressed toward D_6-symmetry and the spin-triplet superconductivity emerges in near the D_6-symmetric system ($t_m = 1$).

In conclusion, we discussed the possibility of spin-triplet superconductivity in a two-dimensional Hubbard model on a triangular lattice within the TOPT. We obtained spin-triplet superconducting states in near the D_6-symmetric system. We pointed out the possibility that our obtained results correspond to the difference between the superconductivity of UNi_2Al_3 and that of UPd_2Al_3.

Numerical computation in this work was carried out at the Yukawa Institute Computer Facility.

References

1) K. Ishida, D. Ozaki, T. Kamatsuka, H. Tou, M. Kyogaku, Y. Kitaoka, N. Tateiwa, N. K.Sato, N. Aso, C. Geibel and F. Steglich: Phys. Rev. Lett.**89** (2002) 037002.
2) Y. Nisikawa and K. Yamada: J. Phys. Soc. Jpn. **71** (2002) 237.
3) T. Nomura and K. Yamada: J. Phys. Soc. Jpn. **69** (2000) 3678.
4) K. Kuroki and R. Arita: Phys. Rev. B **63** (2001) 174507.
5) Y. Nisikawa, H. Ikeda and K. Yamada: J. Phys. Soc. Jpn. **71** (2002) 1140.
6) T. Jujo, S. Koikegami and K. Yamada: J. Phys. Soc. Jpn. **68** (1999) 1331.

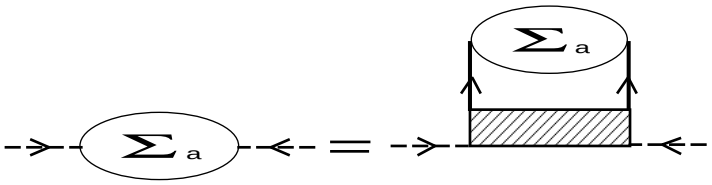

Fig. 1. Éliashberg's equation. The thick line represents Green's function with self-energy correction. The shaded rectangle represents the effective interaction.

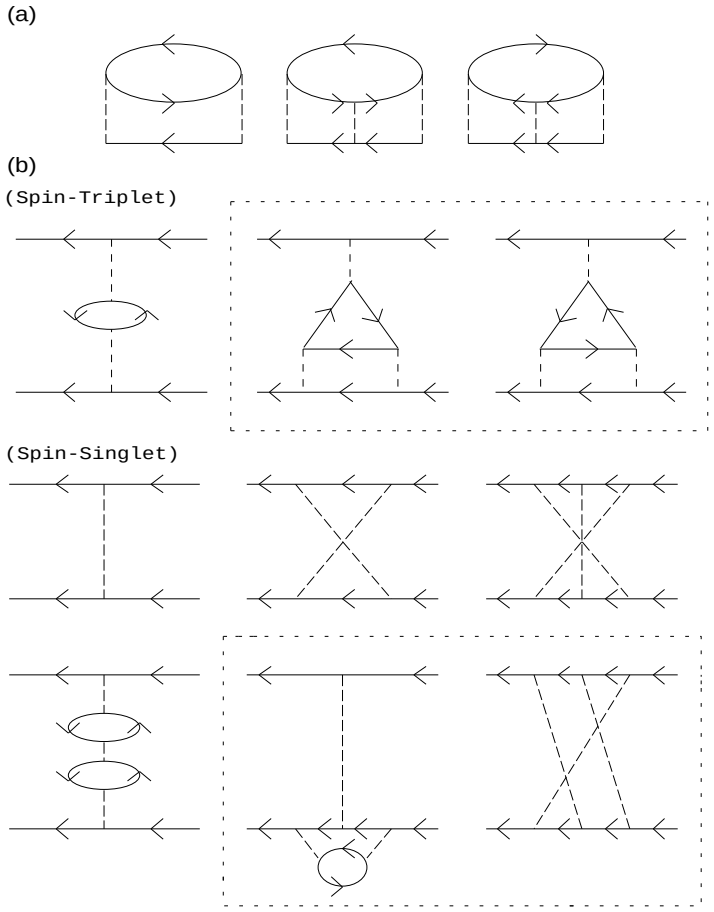

Fig. 2. (a) Feynman diagrams of the normal self-energy up to the third order. (b) Feynman diagrams of the effective interaction up to the third order. Solid and dashed lines correspond to the bare Green's function and the interaction, respectively.

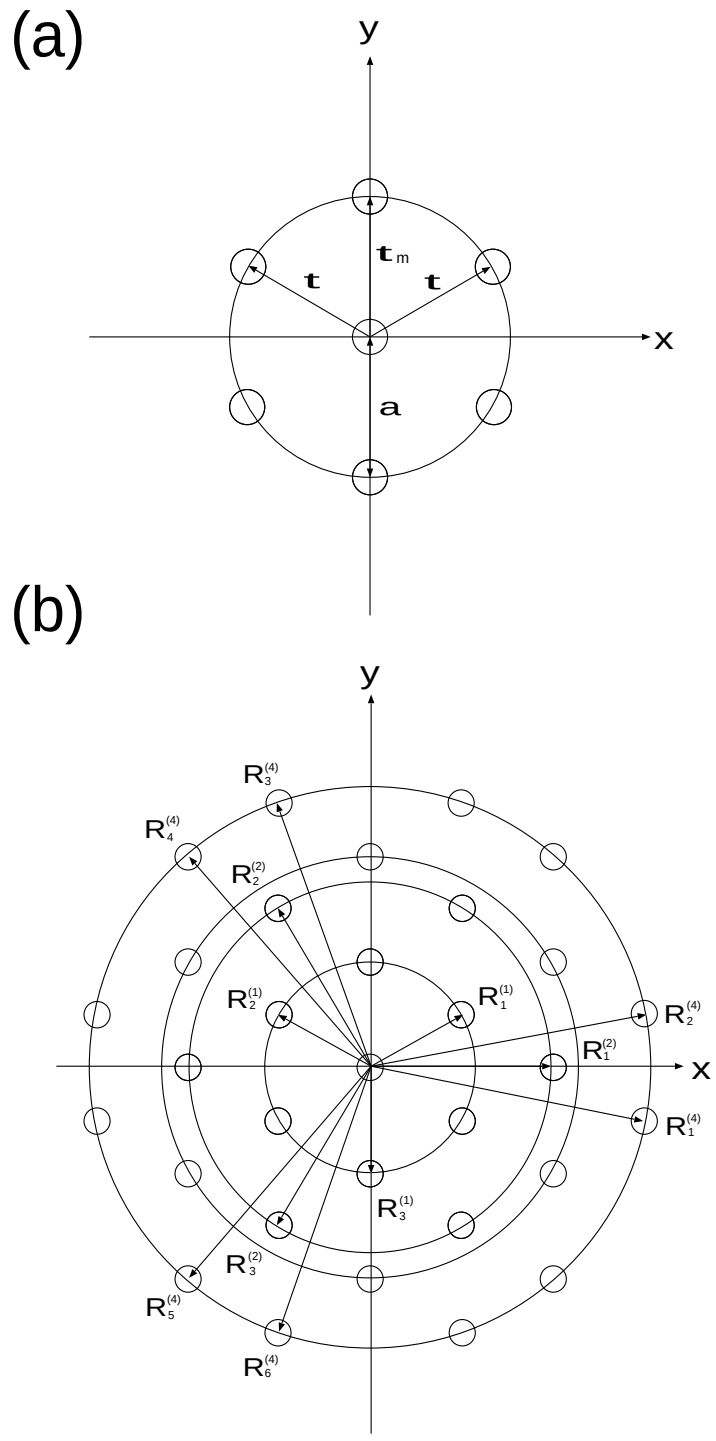

Fig. 3. (a) Hopping integrals with anisotropic nature (D_2-symmetry) on triangular lattice. (b) Labels of basis functions.

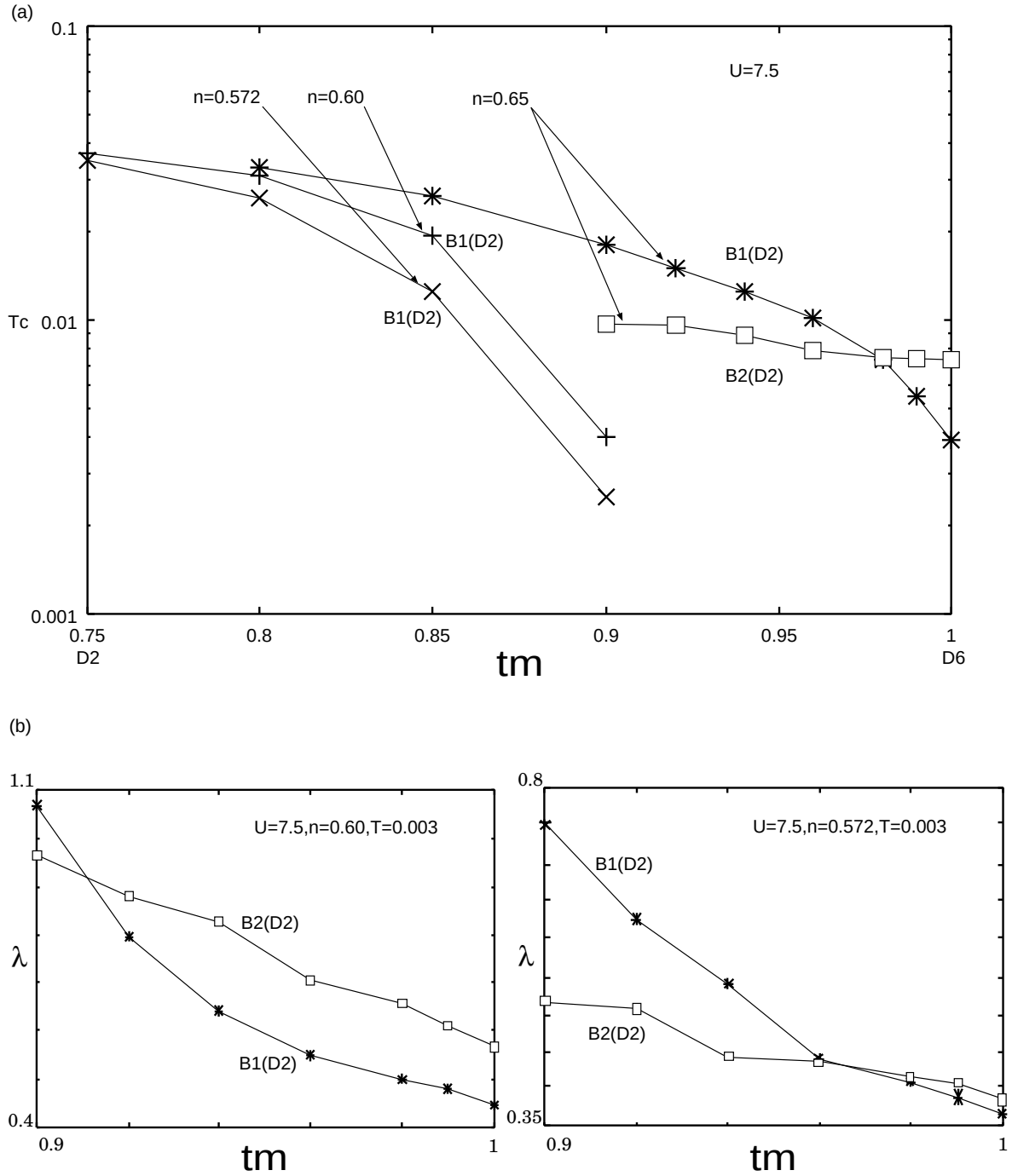

Fig. 4. (a) The calculated T_c is shown as a function of t_m for various electron numbers n per one spin site. (b) The calculated eigenvalue is shown as a function of t_m at $T_{lim} = 0.003$ for $n = 0.572$ and 0.600

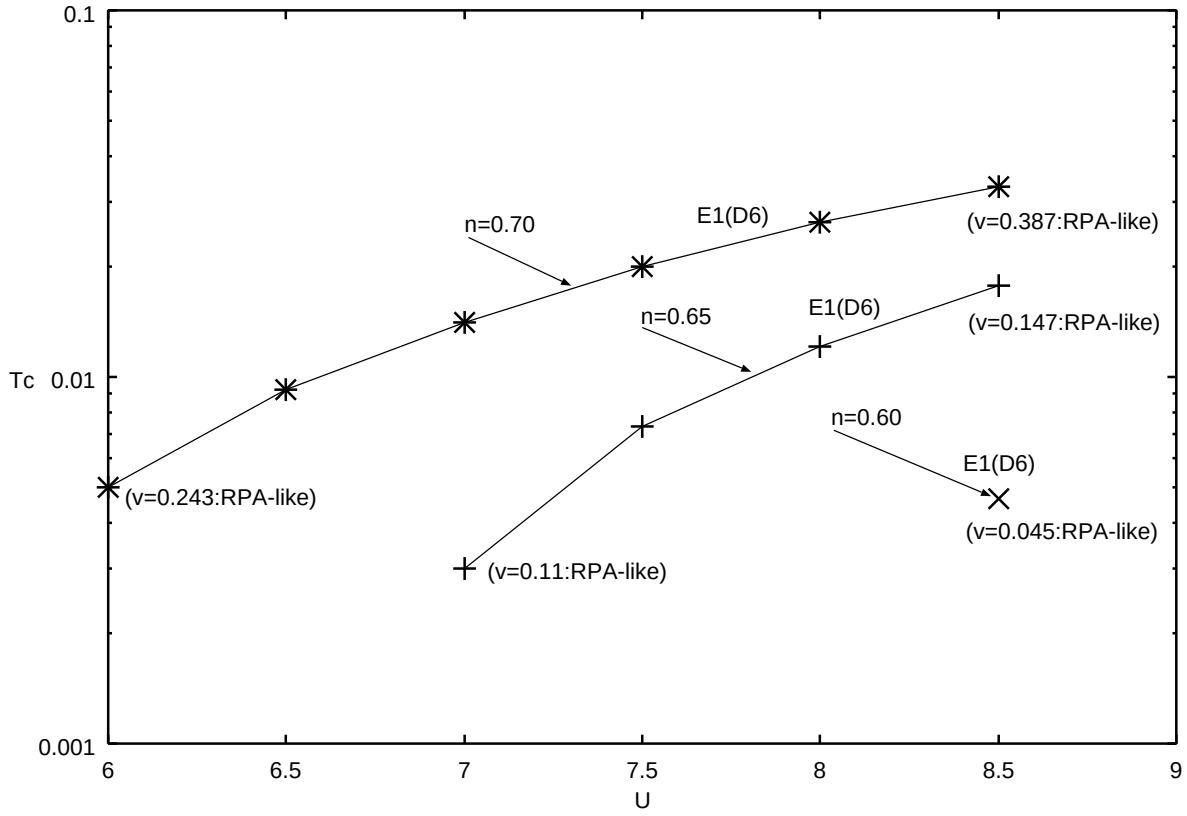

Fig. 5. The calculated T_c is shown as a function of U for various electron numbers n per one spin site." In this figure, (v=***:RPA-like)" means that eigenvalue v calculated by including only the RPA-like diagrams is v=*** at T_c obtained by using the TOPT.